

# **Basic Energy Sciences**

The Office of Science's Basic Energy Sciences (BES) program supports fundamental research in materials sciences and engineering, chemistry, geosciences, and molecular biosciences. In 2001, BES funded research in more than 170 academic institutions located in 49 states and in 13 DOE laboratories located in 9 states. The BES program also supports world-class scientific user facilities, including four synchrotron radiation light sources, three neutron scattering facilities, and four electron-beam micro characterization centers. Annually, 8,000 researchers from academia, industry, and Federal laboratories perform experiments at these facilities. Under construction is the Spallation Neutron Source (SNS), a \$1.4 billion next-generation, neutron-scattering facility.

# **The Opportunity**

In the past century, the triumphs of science, which improved our lives immeasurably, were elegant and simple solutions to complex problems that had puzzled scientists for millennia. We discovered and characterized the atomic building blocks of matter, the elementary excitations in materials, and the fundamentals of chemical reactivity. We used this knowledge to design, synthesize, and characterize simple molecules and to use them as components of alloys, ceramics, and catalysts. The next millennium leads us into a more complex world of research with unprecedented opportunities. Here, large, complicated structures can be designed atom by atom for desired characteristics. Here, also, chemical reactivity can be predicted and controlled. New tools, new understanding, and a developing convergence of the BES-supported disciplines will allow us to ask

# The Challenge

BES support of fundamental research is oriented toward resolving some of the greatest scientific challenges of the 21st Century:

and solve questions that were previously the stuff of science fiction.

Science at the Nanoscale. Can we achieve a fundamental understanding of nanoscale assemblies of materials—structures 1000 times smaller than a human hair? At the nanoscale, materials have properties distinctly different from those with which we are familiar. Lessons learned from many decades of research in chemistry and materials sciences do not apply at the nanoscale and new research must be conducted.

Materials by Design. Can we design materials having predictable and yet often unusual properties? This will require "bottoms-up" atomic and molecular design, the use of nanostructured materials, novel routes for materials synthesis and processing, and parallel fabrication design and construction of multi-component molecular devices and machines having desired properties—optical, mechanical, catalytic, electrical, tribological. These might form the basis of systems such as nanometer-scale chemical factories, molecular pumps, sensors, and self-assembling electronic/photonic devices.

Chemical Reactivity. Can we predict and control chemical reactivity—the making and breaking of chemical bonds to fabricate desired products while minimizing or eliminating unwanted products? The convergence of chemical catalysis and biological catalysis coupled with new, exotic techniques such as laser-based control, may make it possible to control reactivity with a precision found only in nature and to fashion novel products not seen in nature.

#### The Molecular Foundations of Natural Processes.

Can we harness, control, or mimic the exquisite complexity of natural processes? Living organisms represent the most sophisticated use of the elements to create materials and functional complexes through chemical processing. Nature's achievements allow us to set goals for the development of materials and systems with the enhanced properties, including the ability to self-assemble, self-repair, sense, respond, and evolve.

Scaling in Space and Time. Can we develop the tools to visualize and predict phenomena spanning the length scales and time scales of natural phenomena? The challenges are formidable. Spatial scaling involves lengths ranging from that of the atom, to thousands of atoms, to the bulk phase, and, finally, to the macroscale. Temporal scaling involves times ranging from those of chemical reactions (femtoseconds) to geologic times (millennia).

### **Investment Plan**

The BES program will strengthen core competencies to address outstanding scientific challenges. In the areas of nanoscale science, engineering, and technology research, the BES program will expand selected research areas. We will continue to design and begin construction of Nanoscale Science Research Centers, which will provide unique, state-of-the-art nanofabrication and characterization facilities to the scientific community. Also of high priority is continued construction of the SNS to provide the next-generation, short-pulse spallation neutron source for neutron scattering.

### **The Benefits**

Basic research supported by the BES program touches virtually every aspect of energy resources, production, conversion, efficiency, and waste mitigation. Research in materials sciences and engineering leads to the development of materials that improve the efficiency, economy, environmental acceptability, and safety of

energy generation, conversion, transmission, and use. For example, research on toughened ceramics will result in improved high-speed cutting tools, engine turbines, and a host of other applications requiring lightweight, high-temperature materials. Research in chemistry leads to the development of advances such as efficient combustion systems with reduced emissions of pollutants; new solar photo conversion processes; improved catalysts for the production of fuels and chemicals; and better separations and analytical methods for applications in energy processes, environmental remediation, and waste management. Research in



The Spallation Neutron Source is an accelerator-based neutron source being built at Oak Ridge National Laboratory

geosciences contributes to the solution of problems in multiple DOE mission areas, including reactive fluid flow studies to understand contaminant remediation and seismic imaging for reservoir definition. Finally, research in the molecular and biochemical nature of plant growth aids the development of renewable biomass resources. History has taught us that seeking answers to fundamental questions results in a diverse array of practical applications as well as some remarkable revolutionary advances.

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